Modeling to Support Fuel Development for an Advanced Fuel Cycle

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U. S. Nuclear Energy Policy

DOE Actions on Nuclear Waste Management 2008-2009

Advanced Fuel Cycle

More Underground Repositories

Fuel Performance Code
IMF, Cermet, CerCer, Actinide Recycle

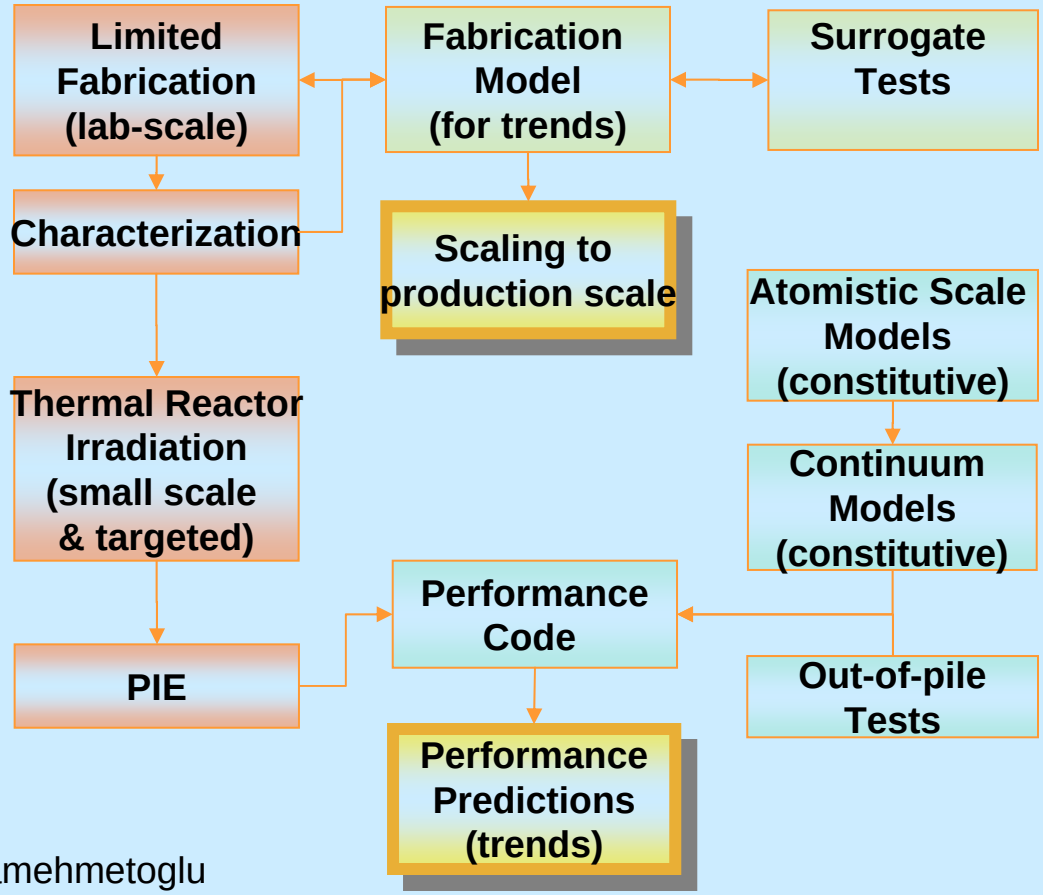
Models, Simulations, and Experimental Validation

First Principles Modeling for Materials of Interest

Materials Science and Engineering of Actinide Alloys and Ceramics

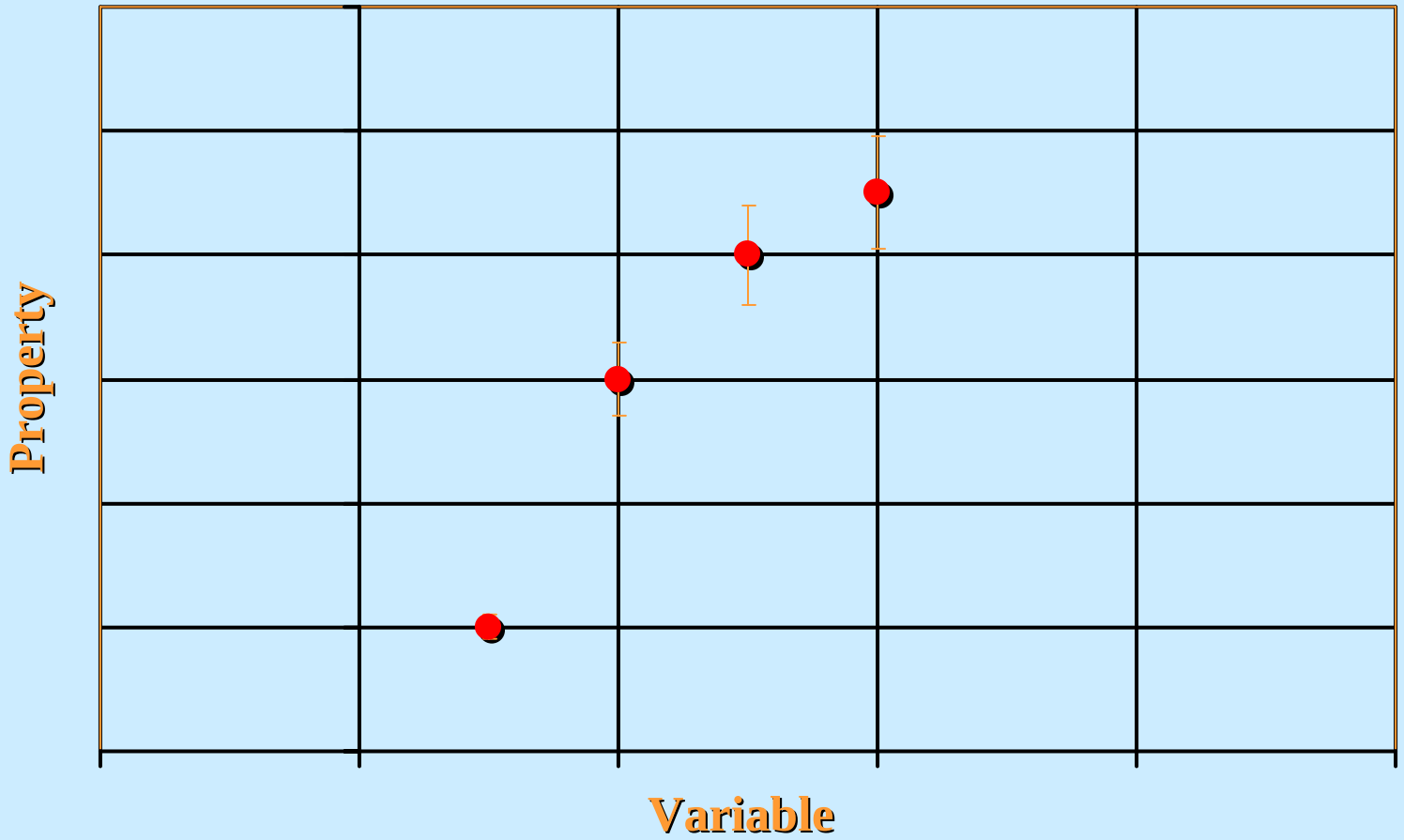
National Security Applications
Non-proliferation

The Role of Models and Simulations in AFCI*

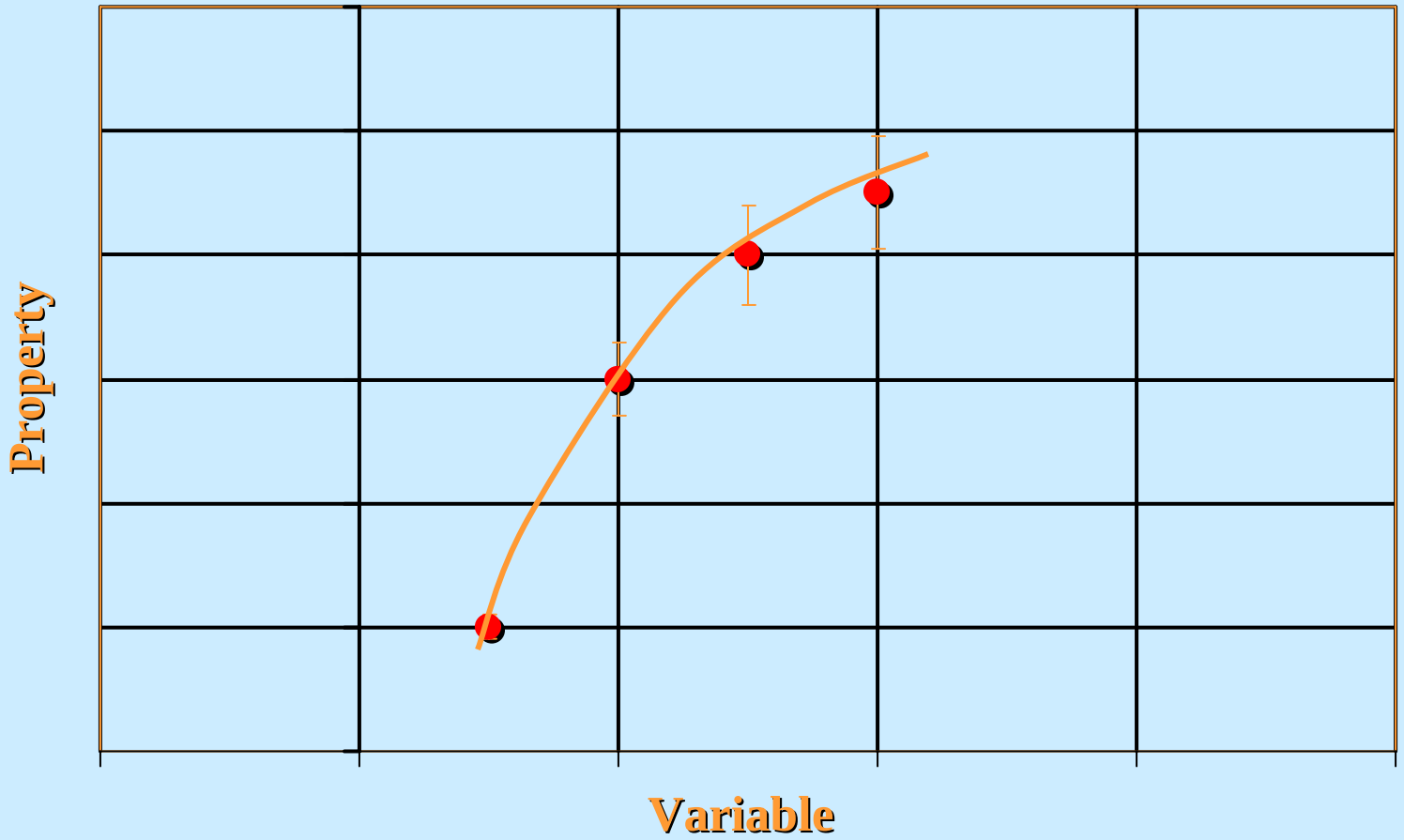


*Courtesy of Kemal Pasamehmetoglu

Replacing Empirical-Based Models



Replacing Empirical-Based Models



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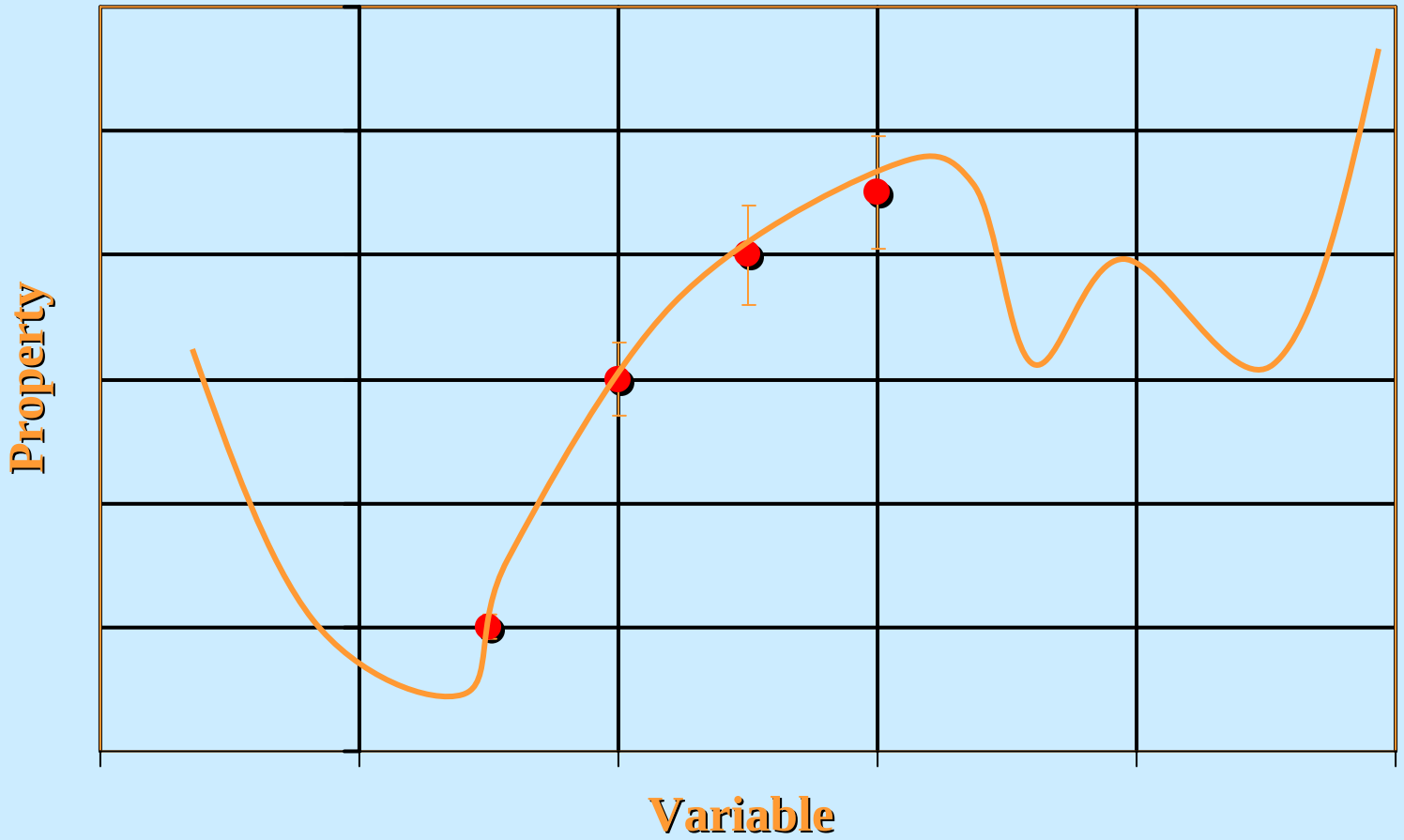
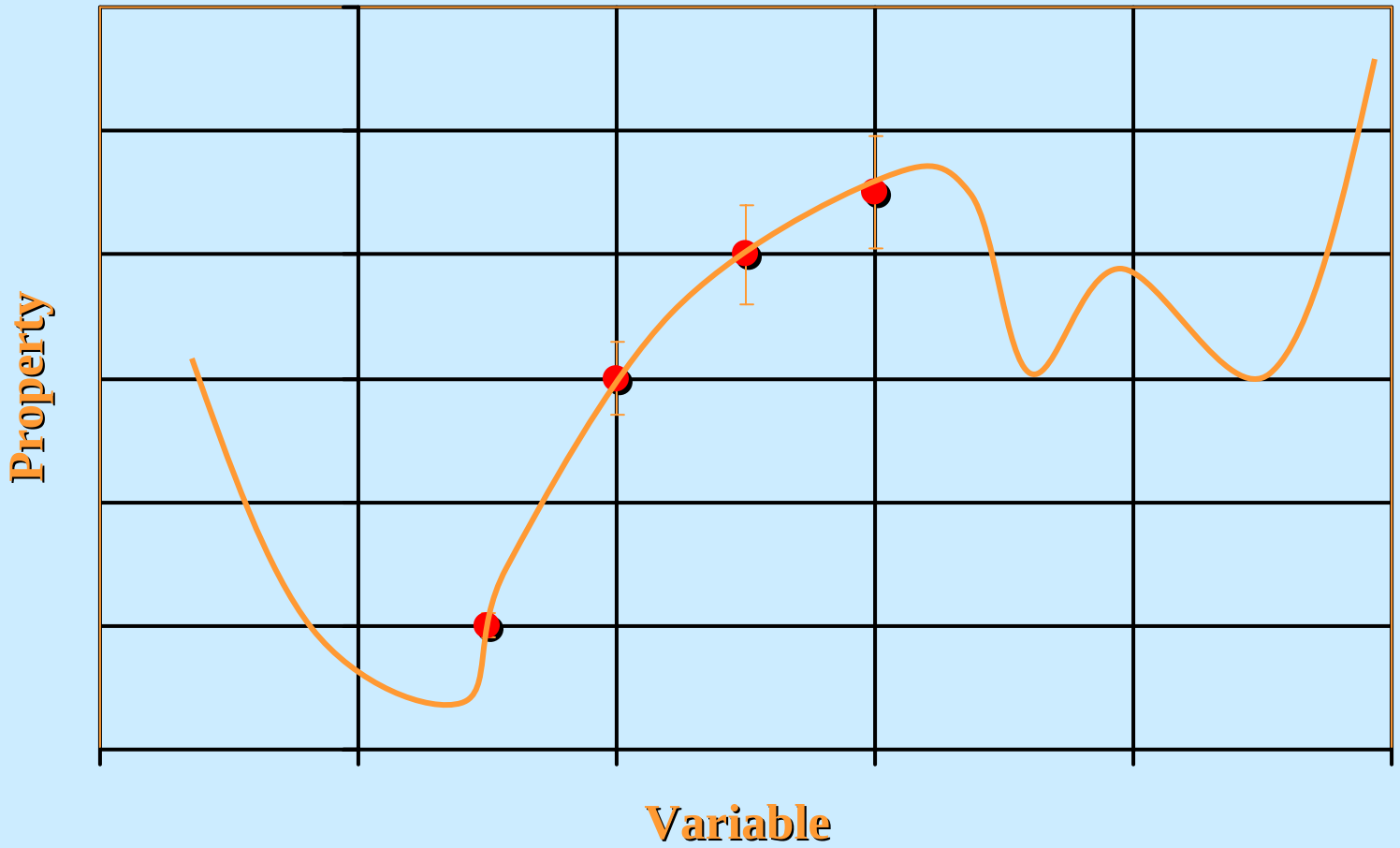


Replacing Empirical-Based Models



Extrapolation of Empirical-Based models can be dangerous!

Current Fuel Performance Codes

- **COMETHE** (Belgonucleaire, Belgium)
- **COPERNIC** (FRAMATOME, Germany)
- **ENIGMA** (British Energy, BNFL, UK)
- **FALCON** (EPRI, USA)
- **FRAPCON** (PNNL, USA)
- **FRAPTRAN** (PNNL, USA)
- **LIFE** (ANL, USA)
- **MACROS** (SCK-CEN, Belgium)
- **ORIGEN** (ORNL, USA)
- **PARFUME** (INEEL, USA)
- **SPHERE** (PSI, Switzerland)
- **TRANSURANUS** (ITU, Germany)

Drawbacks of Current Fuel Performance Codes

Design

- Not object oriented
- No parallel processing capability
- Not applicable for fuel processing

Models

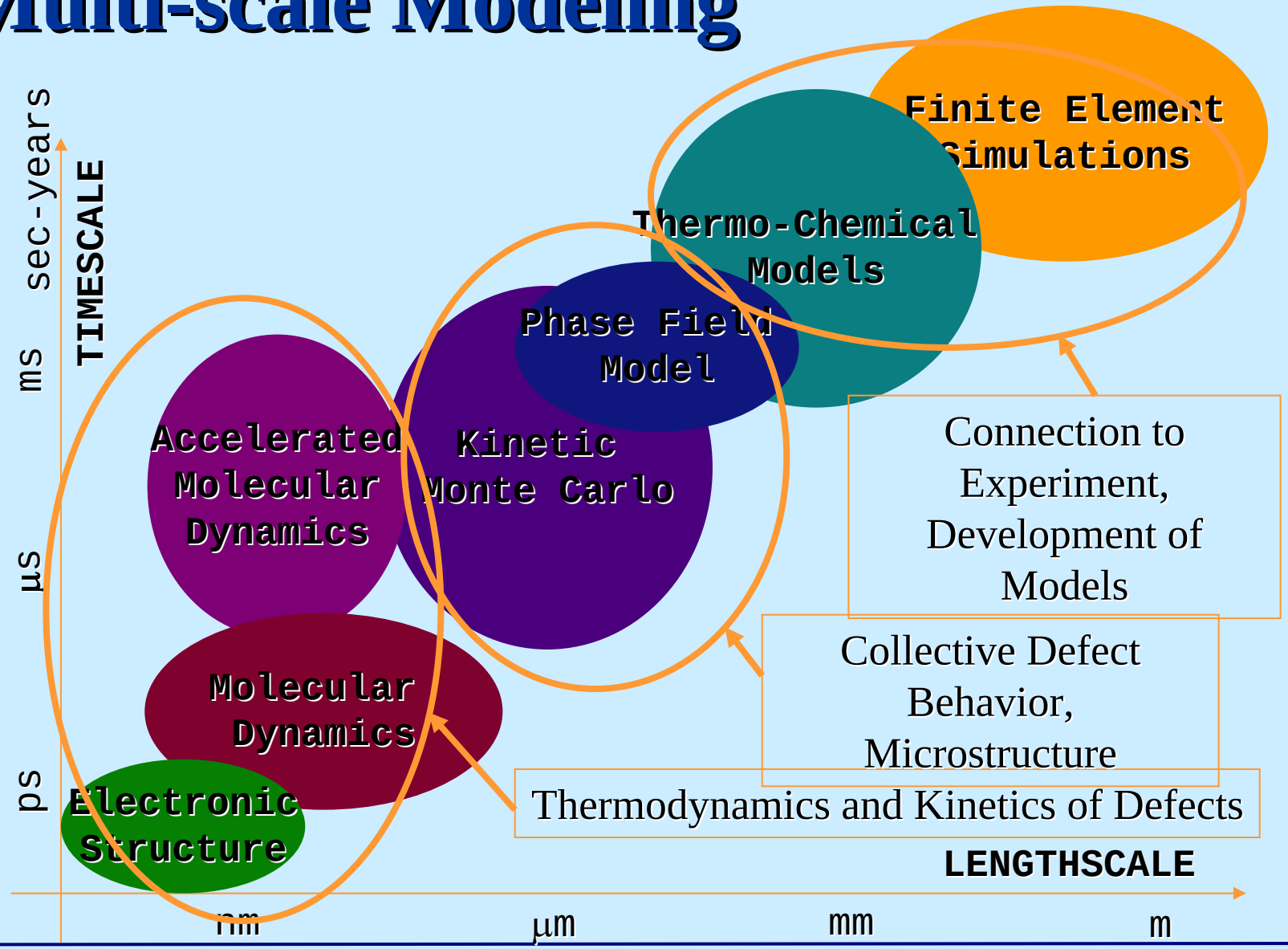
- Empirical correlations, unreliable extrapolations
- Material specific (limited materials)
- No uncertainty evaluation

ASCI*-Type Program for Nuclear Fuels
Software Engineering Steps

- Scope and Objectives
- Requirements
- Risk Assessment
- Code Design & Development
- Prototype
- Implementation
- Testing (verification + validation)
- Release
- User Group

*ASCI = Advanced Simulation and Computing Initiative (DOD/DOE funded)

Multi-scale Modeling



Advanced Models, Simulations, and Fuel Performance Code

Advanced Fuel Performance Code

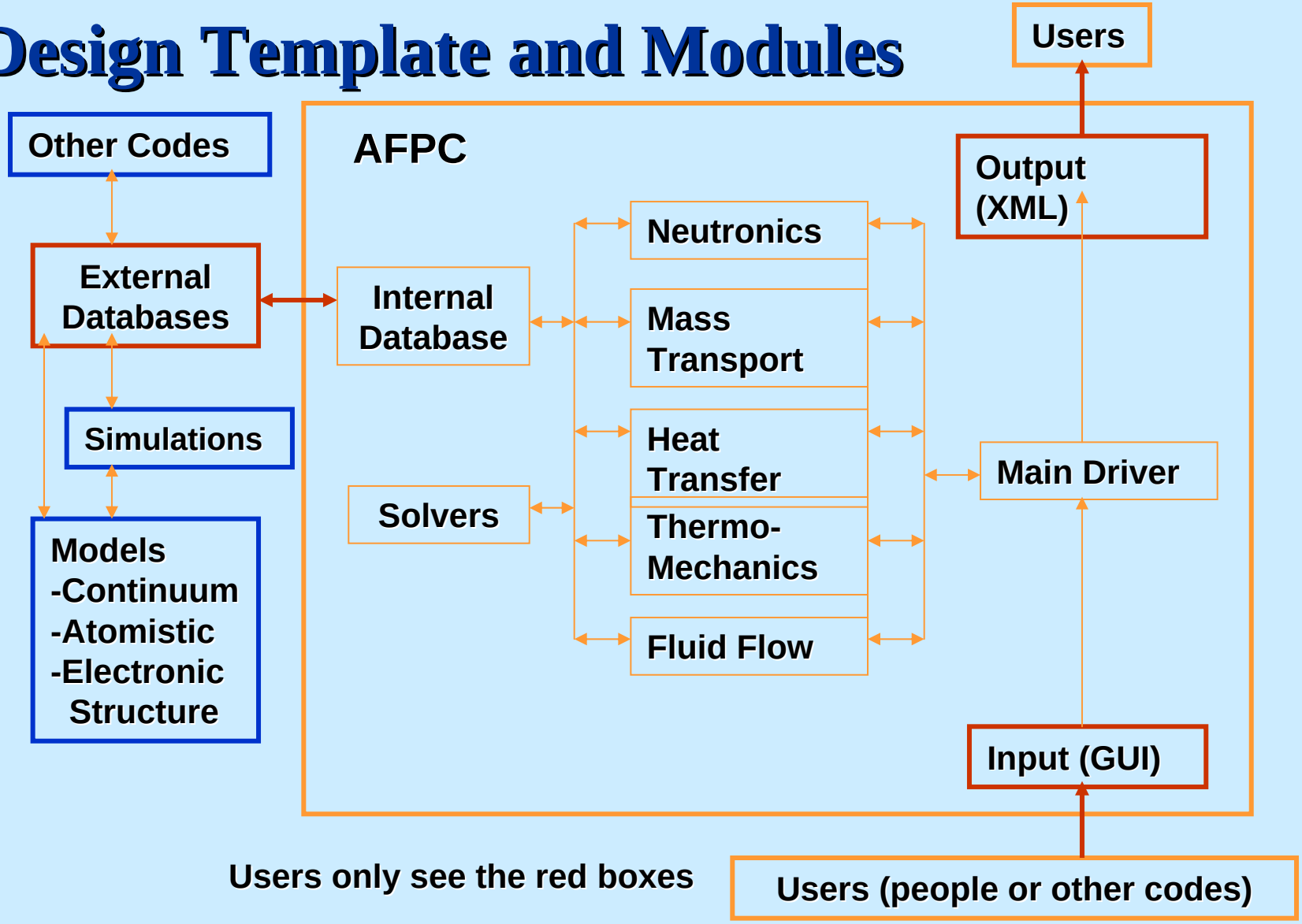
- Fission products kinetics and concentration
- Heat transfer simulations
- Diffusion of species (gas and fission products) simulations
- Chemical reactions simulations

Incorporation of the Advanced Models

Advanced Models and Simulations

- Continuum-scale: Thermo-mechanical properties
- Meso-scale: Microstructural evolution, Species mobility
- Atomic-scale: Defect formation free energy, Irradiation effects
- Electronic Structure: Structural stability, elastic constants

Advanced Fuel Performance Code Design Template and Modules



Summary

- Current fuel performance codes limited to experimental data.
- Codes are currently too material specific, not of use to AFCI program for most part.
- Codes need broader applications to fuel processing, in addition to fuel performance.
- Can build upon success of ASCI program.